

Initial Temperature-Dependent Validation of an ENDF/B-VIII.1 H-H₂O TSL

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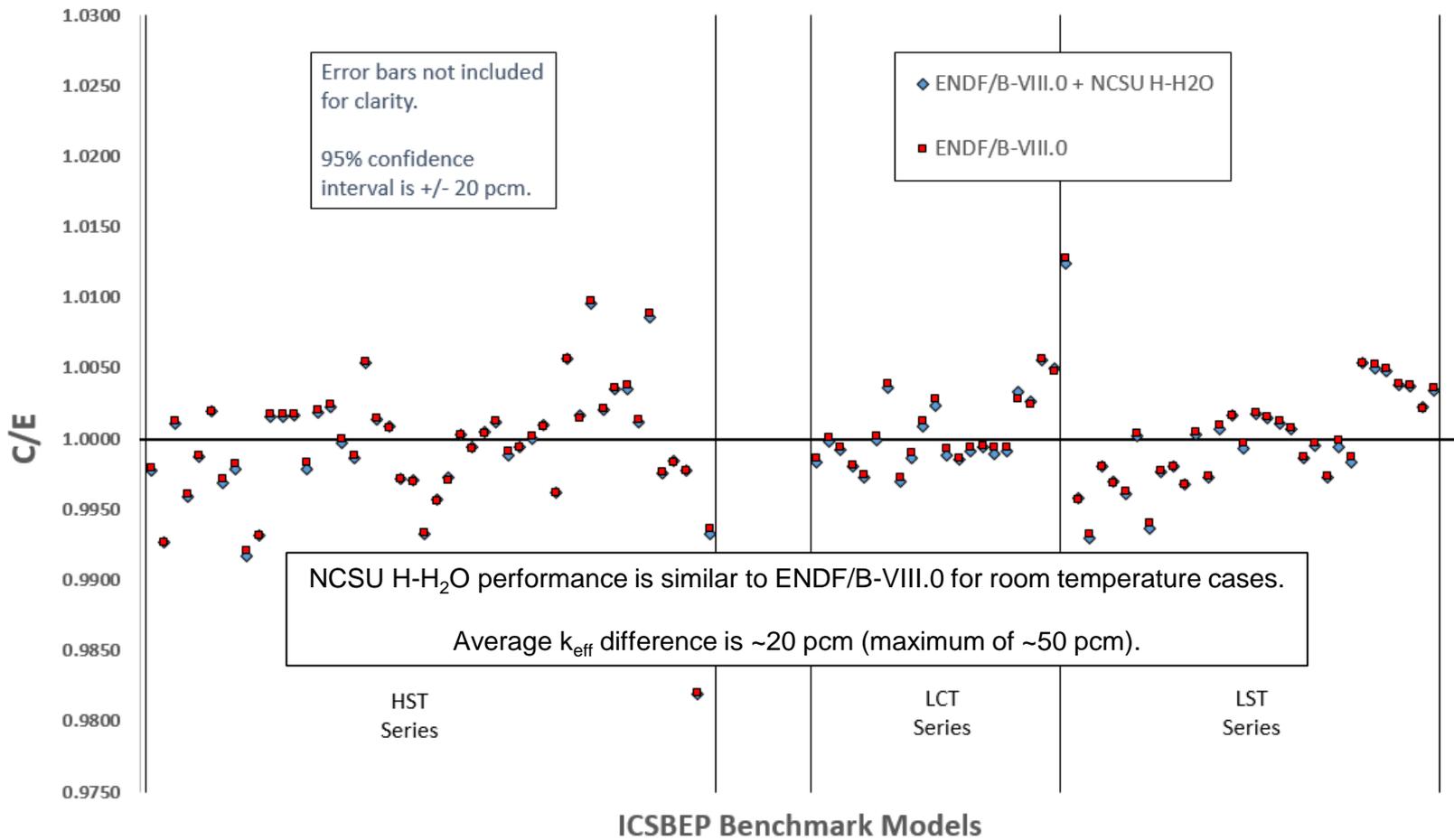


ENDF/B-VIII.1 H-H₂O TSL

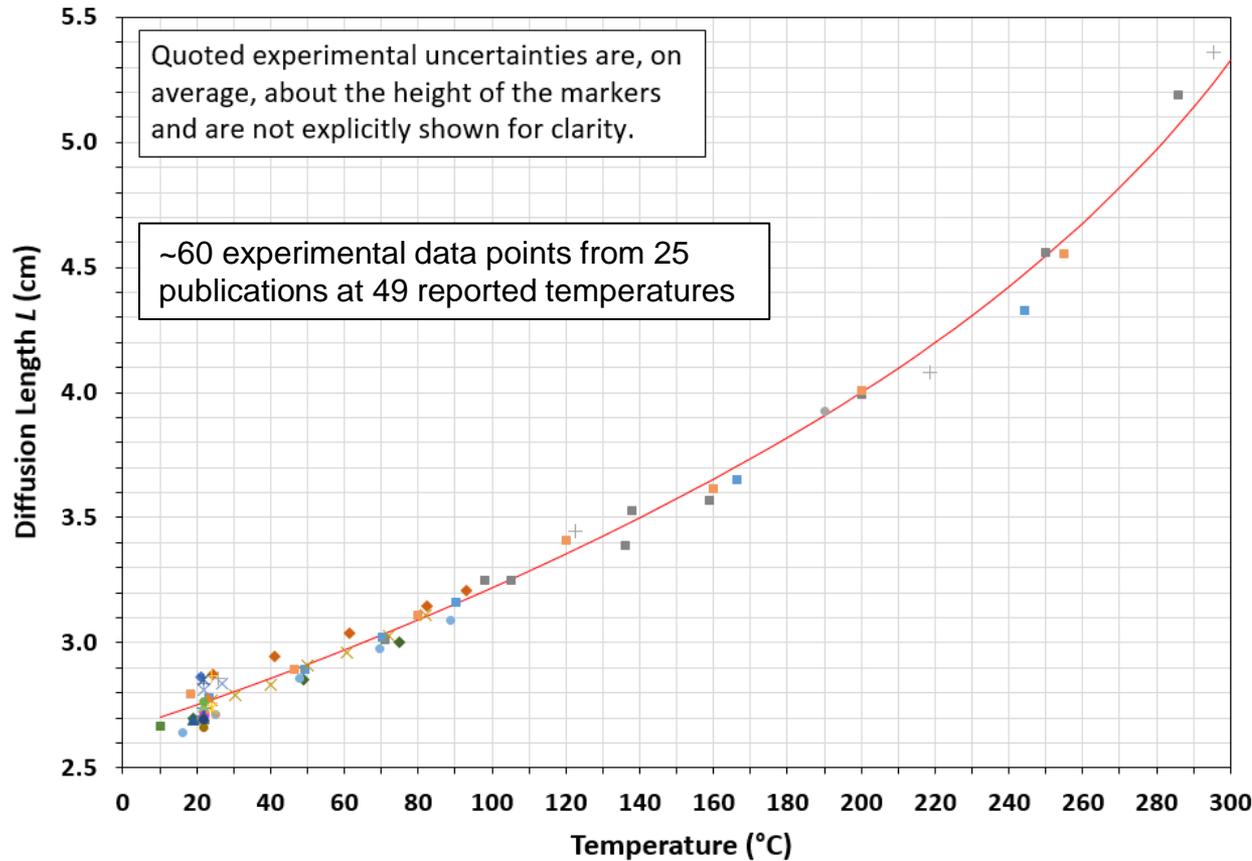
Motivation, Experimental Data, and Validation

- The proposed TSL is developed by North Carolina State University (NCSU) using LAMMPS molecular dynamics (MD) simulations optimized based on experimental thermophysical properties over a wide range of T .
- Refinement of the H-H₂O thermal scattering law (TSL) at elevated temperatures is of interest for operating reactor conditions. Validation historically focuses on room temperature performance (e.g., ICSBEP benchmarks).
- H-H₂O TSL evaluations depend on separately-defined temperature-dependent phonon and diffusion information. Validation at one T does not provide direct assurance of acceptable performance at a different T .
- Elevated-temperature pulsed-neutron die-away (PNDA) and static spatial flux decay simulations show improvement in prediction of the thermal diffusion length against experimental data compared to ENDF/B-VII.1 and ENDF/B-VIII.0 TSLs.

Selected ICSBEP Benchmarks (k_{eff} C/E) (Room Temperature)

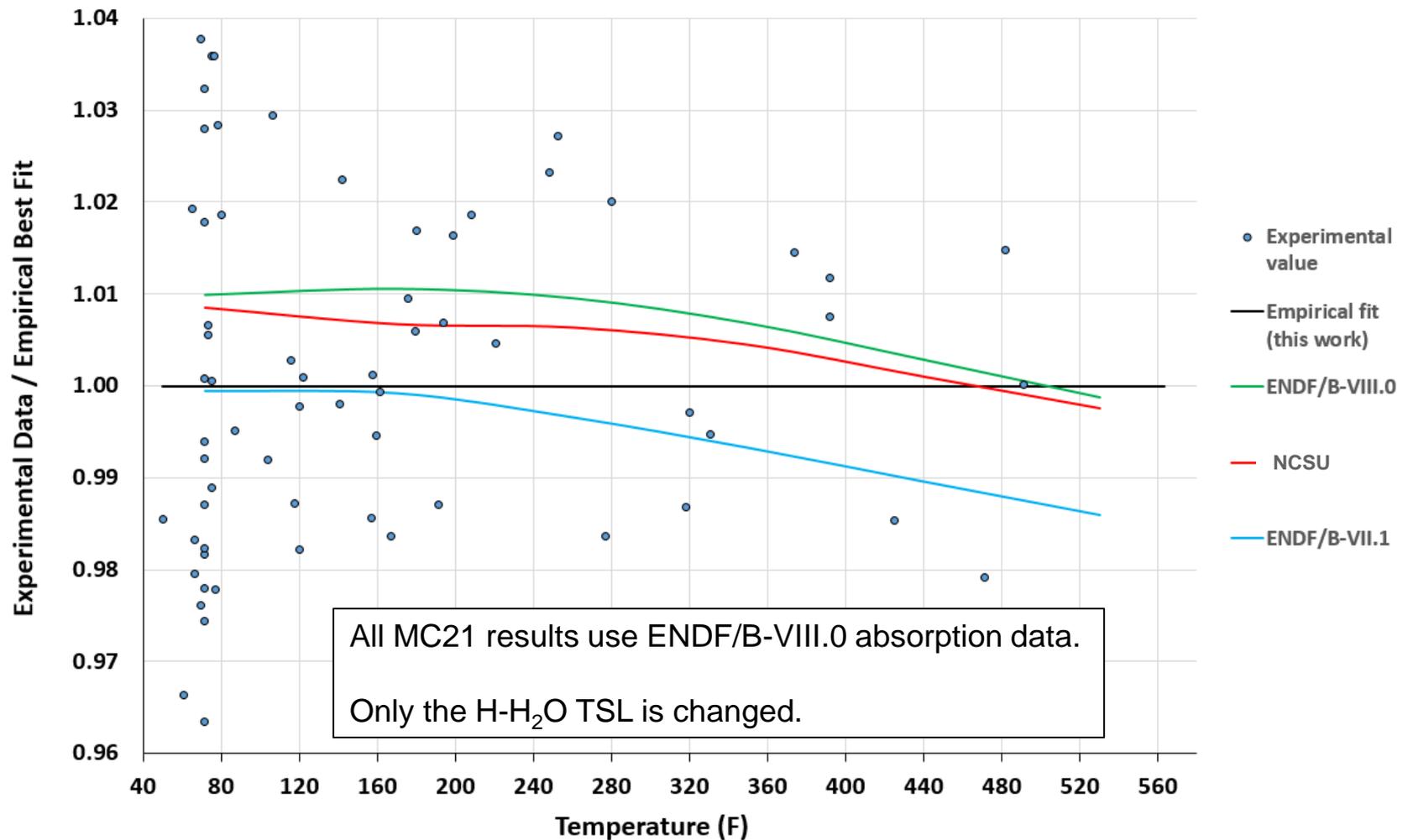


Compilation of Historical Thermal Neutron Diffusion Length (L) Measurements for Water



- × Lopez, Beyster (1962)
- Von Dardel, Sjöstrand (1954)
- ▲ Antonov et al. (1956)
- Bracci, Coceva (1956)
- ◆ Dio, Schopper (1958)
- + Dio (1958)
- ▲ Kuchle (1960)
- Antonov et al. (1962)
- Kobayashi et al. (1966)
- Reier, De Juren (1961)
- Besant, Grant (1966)
- ◆ Russell et al. (1962)
- Parks et al. (1968)
- + Rockey, Skolnik (1960)
- Csikai et al. (1961)
- × Besant, Grant (1964)
- ▲ Wilson et al. (1944)
- Wright, Frost (1956)
- × Sisk (1951)
- ◆ Heintze (1956)
- De Juren, Rosenwasser (1953)
- ▲ Barkov et al. (1957)
- Campbell, Stelson (1956)
- + Ballowe (1962)
- × Scott et al. (1954)
- Empirical fit (this work)

MC21 Diffusion Length Results in Empirical Ratio Space



Conclusions / Future Work

- The thermal diffusion length L is an integral property of a single material's absorption and scattering cross sections (both differential and integral). No other neutron reactions or materials are involved.
- The MC21-calculated L for water is consistent with the spread of experimental data and is sufficiently sensitive to different H-H₂O TSL physics models to use the method as a TSL integral performance benchmark.
- Modern high-quality diffusion experiments at elevated T would allow direct low-cost physics benchmarking of water TSLs when public elevated- T critical benchmarks are limited. RPI and LLNL are developing a PNDA capability in coordination with NNL.